

# **Numerical Uncertainty Analysis for Computational Fluid Dynamics using Student T Distribution – Application of CFD Uncertainty Analysis compared to Exact Analytical Solution**

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## **Extended Abstract**

**Computational Fluid Dynamics (CFD) is the standard numerical tool used by Fluid Dynamists to estimate solutions to many problems in academia, government, and industry. CFD is known to have errors and uncertainties and there is no universally adopted method to estimate such quantities. This paper describes an approach to estimate CFD uncertainties strictly numerically using inputs and the Student-T distribution. The approach is compared to an exact analytical solution of fully developed, laminar flow between infinite, stationary plates. It is shown that treating all CFD input parameters as oscillatory uncertainty terms coupled with the Student-T distribution can encompass the exact solution.**

## **Nomenclature**

|                                           |                                        |
|-------------------------------------------|----------------------------------------|
| <b>a</b>                                  | = channel width                        |
| <b><math>\delta_D</math></b>              | = experimental error                   |
| <b><math>\delta_{\text{input}}</math></b> | = input error                          |
| <b><math>\delta_{\text{model}}</math></b> | = modeling error                       |
| <b><math>\delta_{\text{num}}</math></b>   | = numerical error                      |
| <b><math>\delta_s</math></b>              | = simulated error                      |
| <b>D</b>                                  | = experimental value                   |
| <b><math>dp/dx</math></b>                 | = pressure gradient                    |
| <b><math>\epsilon_{21}</math></b>         | = solution changes medium to fine grid |

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|                   |                                                       |
|-------------------|-------------------------------------------------------|
| $\epsilon_{32}$   | = solution changes coarse to medium grid              |
| $e_a^{21}$        | = extrapolated error                                  |
| $E$               | = comparison error                                    |
| $GCI_{fine}^{21}$ | = grid convergence index                              |
| $h$               | = representative grid size                            |
| $p$               | = observed order                                      |
| $R_k$             | = convergence parameter                               |
| $r_{21}$          | = ratio of grid sizes between grid 1 and 2            |
| $r_{32}$          | = ratio of grid sizes between grid 3 and 2            |
| $S$               | = simulated result                                    |
| $S_{k1}$          | = solution variable for fine grid                     |
| $S_{k2}$          | = solution variable for medium grid                   |
| $S_{k3}$          | = solution variable for coarse grid                   |
| $S_{ext}^{21}$    | = extrapolated solution variable                      |
| $S_L$             | = lowest solution variable                            |
| $S_U$             | = highest solution variable                           |
| $U_{oscillatory}$ | = uncertainty for oscillatory portion of the solution |
| $U_{monotonic}$   | = uncertainty for monotonic portion of the solution   |
| $u_{input}$       | = input uncertainty                                   |
| $u_D$             | = experimental uncertainty                            |
| $u_{num}$         | = numerical uncertainty                               |
| $u_{val}$         | = validation uncertainty                              |
| $\mu$             | = viscosity                                           |

## I. Introduction

CFD in many problems is the optimum balance between cost and accuracy. However, a comprehensive approach for verification using test data is needed for full validation. With shrinking budgets in all areas of aerospace industry, CFD is commonly used without proper verification and validation. This paper couples traditional

uncertainty analysis with the Student-T distribution to estimate a numerical uncertainty without using test data. The results are compared to the exact analytical solution of fully developed, laminar flow between infinite, stationary plates.

A thorough literature review was performed by the authors in AIAA-2013-0258<sup>1</sup> and it was determined that the current state of the art for CFD uncertainty analysis is the ASME Standard for Verification and Validation in Computational Fluid Dynamics and Heat Transfer<sup>2</sup>. The standard outlines a validation approach using experimental errors, modeling assumptions, simulation inputs, and numerical solutions of equations. The error,  $E$ , and validation standard uncertainty  $u_{val}$ , can be defined and conclusions drawn about whether the model is properly verified. This paper outlines a method to estimate the numerical uncertainty without using test data and shows the differences between the proposed methodology and the ASME Standard.

## II. Methodology of ASME V&V 20-2009

A schematic showing the nomenclature and an overview of the validation process is shown in Figure 1<sup>2</sup>. The left side of the figure describes the terminology and the right side describes the validation process.

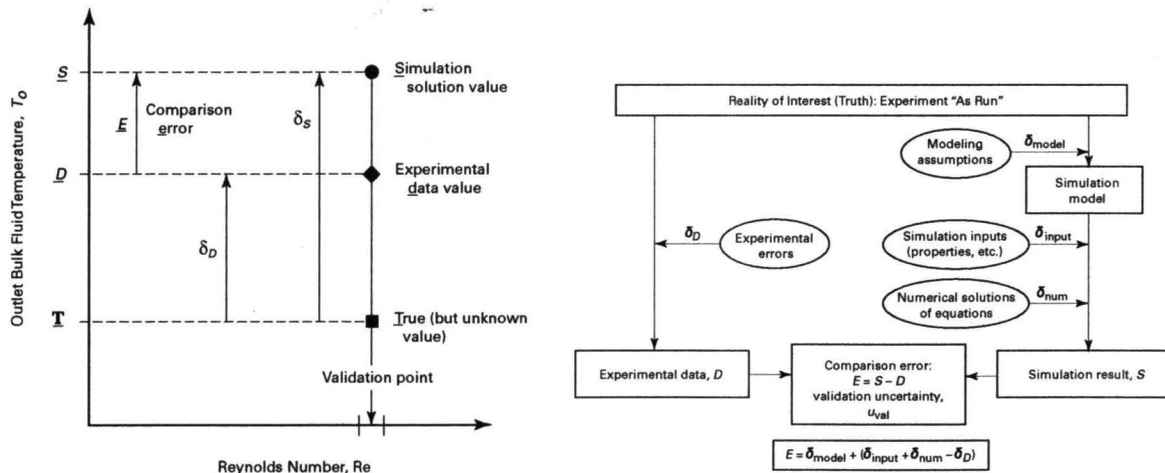


Figure 1: Schematic of nomenclature and Overview of Validation Process<sup>2</sup>

The methodology is as follows. The validation comparison error,  $E$ , is the difference between the simulated result,  $S$ , and the experimental value,  $D$ <sup>2</sup>. The goal is to characterize the interval modeling error,  $\delta_{model}$ . The coverage factor,  $k$ , used to provide a given degree of confidence (ie 90% assuming a uniform distribution,  $k=1.65$ )<sup>2</sup>.

The standard also outlines procedures to calculate numerical uncertainty,  $u_{num}$ , the uncertainty in the simulated result from input parameters,  $u_{input}$ , and the experimental uncertainty,  $u_D$ <sup>2</sup>.

$$\delta_{model} \varepsilon[E - u_{val}, E + u_{val}] \quad (1)$$

$$E = S - D \quad (2)$$

$$u_{val} = k (\sqrt{u_{num}^2 + u_{input}^2 + u_D^2}) \quad (3)$$

$U_{num}$  is calculated using a Richardson's Extrapolation approach and defined as a five-step procedure<sup>2</sup>.

Step 1, calculate representative grid size,  $h$  as shown in equation 4.

$$\begin{aligned} h_1 &= \left( \frac{\text{Total Volume}}{\text{total number of cells in fine grid}} \right)^{\frac{1}{3}} \\ h_2 &= \left( \frac{\text{Total Volume}}{\text{total number of cells in medium grid}} \right)^{\frac{1}{3}} \\ h_3 &= \left( \frac{\text{Total Volume}}{\text{total number of cells in coarse grid}} \right)^{\frac{1}{3}} \end{aligned} \quad (4)$$

Step 2 is to select three significantly ( $r > 1.3$ ) grid sizes and computer the ratio as shown in equation 5<sup>2</sup>.

$$\begin{aligned} r_{21} &= \frac{h_2}{h_1} \\ r_{32} &= \frac{h_3}{h_2} \end{aligned} \quad (5)$$

Step 3 is to calculate the observed order,  $p$ , as shown in equation 6<sup>2</sup>. This equation must be solved iteratively.

$$\begin{aligned} \varepsilon_{21} &= S_{k2} - S_{k1} \\ \varepsilon_{32} &= S_{k3} - S_{k2} \\ p &= \left[ \frac{1}{\ln(r_{21})} \right] * \left[ \ln \left( \frac{\varepsilon_{32}}{\varepsilon_{21}} \right) + \ln \left( \frac{r_{21}^{p-\text{sign}(\frac{\varepsilon_{32}}{\varepsilon_{21}})}}{r_{32}^{p-\text{sign}(\frac{\varepsilon_{32}}{\varepsilon_{21}})}} \right) \right] \end{aligned} \quad (6)$$

Step 4 is to calculate the extrapolated values as shown in equation 7<sup>2</sup>.

$$\begin{aligned} S_{ext}^{21} &= \frac{(r_{21}^p * S_{k1} - S_{k2})}{(r_{21}^p - 1)} \\ e_a^{21} &= \frac{(S_{k1} - S_{k2})}{(S_{k1})} \end{aligned} \quad (7)$$

Step 5 is to calculate the fine grid convergence index and numerical uncertainty as shown in equation 8<sup>2</sup>. This approached used a factor of safety of 1.25 and assumed that the distribution is Gaussian about the fine grid, 90 % confidence.

$$GCI_{fine}^{21} = \frac{1.25 * e_a^{21}}{(r_{21}^p - 1)}$$

$$u_{num} = \frac{GCI_{fine}^{21}}{1.65} \quad (8)$$

$U_{input}$  is calculated using a Taylor Series expansion in parameter space<sup>2</sup>.

$$u_{input} = \sqrt{\sum_{i=1}^n \left( \frac{\partial S}{\partial x_i} u_{xi} \right)^2} \quad (9)$$

$U_D$  is calculated using test uncertainty methodology as defined in the standard<sup>2</sup>. The purpose of this paper is to show an estimate of numerical uncertainty without test data. The reader is referred to the ASME standard for further information.

### III. Proposed Methodology without Test Data

Convergence studies require a minimum of three solutions to evaluate convergence with respect to an input parameter<sup>3</sup>. Consider the situation for 3 solutions corresponding to fine  $S_{k1}$ , medium  $S_{k2}$ , and coarse  $S_{k3}$  values for the  $k$ th input parameter<sup>3</sup>. Solution changes  $\epsilon$  for medium-fine and coarse-medium solutions and their ratio  $R_k$  are defined by<sup>3</sup>:

$$\epsilon_{21} = S_{k2} - S_{k1}$$

$$\epsilon_{32} = S_{k3} - S_{k2}$$

$$R_k = \epsilon_{21} / \epsilon_{32} \quad (10)$$

Three convergence conditions are possible<sup>3</sup>:

- (i) Monotonic convergence:  $0 < R_k < 1$
  - (ii) Oscillatory convergence:  $R_k < 0$
  - (iii) Divergence:  $R_k > 1$
- (11)

The methodology outlined in ASME V&V-2009<sup>2</sup> assumes monotonic convergence criteria for  $u_{num}$ . Further increasing the grid does not always provide a monotonically increasing result. This is shown in AIAA-2013-0258<sup>1</sup>. The proposed methodology is to treat all input parameters including the grid as an oscillatory convergence study. The uncertainty for cells with oscillatory convergence, using the following method outlined by Stern, Wilson, Coleman, and Paterson<sup>3</sup>, can be calculated as follows in equation 12.  $S$  is the simulated result. For this case it is the upper velocity  $S_U$  and the lower velocity  $S_L$ .

$$U_{Oscillatory} = \left| \frac{1}{2}(S_U - S_L) \right| \quad (12)$$

The proposed methodology as compared to the ASME Standard is as follows. If there is no experimental data,  $D=0$ ,  $\delta_D=0$ , and  $u_D=0$ .

$$E = S - D = S$$

$$\delta S = S - T$$

$$E = S - D = T + \delta S - (T + \delta_D) = \delta_S - \delta_D = \delta_S$$

$$u_{val} = k (\sqrt{u_{num}^2 + u_{input}^2 + u_D^2}) = u_{val} = k (\sqrt{u_{num}^2 + u_{input}^2}) \quad (13)$$

$$\text{Report the simulated result, } S \text{ as } S \pm u_{val} \quad (14)$$

Also instead of assuming a gauss-normal distribution as in the standard when including test data, the k-value will come from the Student-T distribution as shown in Table 1.

Table 1 – Student – T Distribution, k Values

| Number of Cases | Degrees of Freedom | Confidence 90% |
|-----------------|--------------------|----------------|
| 2               | 1                  | 6.314          |
| 3               | 2                  | 2.92           |
| 4               | 3                  | 2.353          |
| 5               | 4                  | 2.132          |
| 6               | 5                  | 2.015          |
| 7               | 6                  | 1.943          |
| 8               | 7                  | 1.895          |
| 9               | 8                  | 1.86           |
| 10              | 9                  | 1.833          |
| 11              | 10                 | 1.812          |
| 12              | 11                 | 1.796          |
| 13              | 12                 | 1.782          |
| 14              | 13                 | 1.771          |
| 15              | 14                 | 1.761          |
| 16              | 15                 | 1.753          |
| 17              | 16                 | 1.746          |
| 18              | 17                 | 1.74           |
| 19              | 18                 | 1.734          |
| 20              | 19                 | 1.729          |
| 21              | 20                 | 1.725          |
| 22              | 21                 | 1.721          |
| 23              | 22                 | 1.717          |
| 24              | 23                 | 1.714          |
| 25              | 24                 | 1.711          |
| 26              | 25                 | 1.708          |
| 27              | 26                 | 1.706          |
| 28              | 27                 | 1.703          |
| 29              | 28                 | 1.701          |
| 30              | 29                 | 1.699          |
| 31              | 30                 | 1.697          |
| 41              | 40                 | 1.684          |
| 51              | 50                 | 1.676          |
| 61              | 60                 | 1.671          |
| 81              | 80                 | 1.664          |
| 101             | 100                | 1.66           |
| 121             | 120                | 1.658          |
| infy            | infy               | 1.645          |

#### IV. Fully Developed Laminar Flow Between Stationary Parallel Plates

Fully developed laminar flow between stationary, parallel plates is an exact solution to the Navier-Stokes Equations as derived in “Introduction to Fluid Mechanics”<sup>4</sup>. The width of the channel is (a).

$$u = \frac{a^2}{2\mu} \left( \frac{\partial P}{\partial x} \right) \left[ \left( \frac{y}{a} \right)^2 - \left( \frac{y}{a} \right) \right] \quad (14)$$

A CFD model of this problem was created in FLUENT. The fluid is air. Table 2 outlines the parameters used.

Table 2 – Parameters

|                           |            |
|---------------------------|------------|
| a (m)                     | 0.1        |
| rho (kg/m <sup>3</sup> )  | 1.225      |
| mu (Ns/m <sup>2</sup> )   | 0.00001789 |
| dp/dx (N/m <sup>3</sup> ) | -0.000400  |

The exact solution is shown in Figure 1.

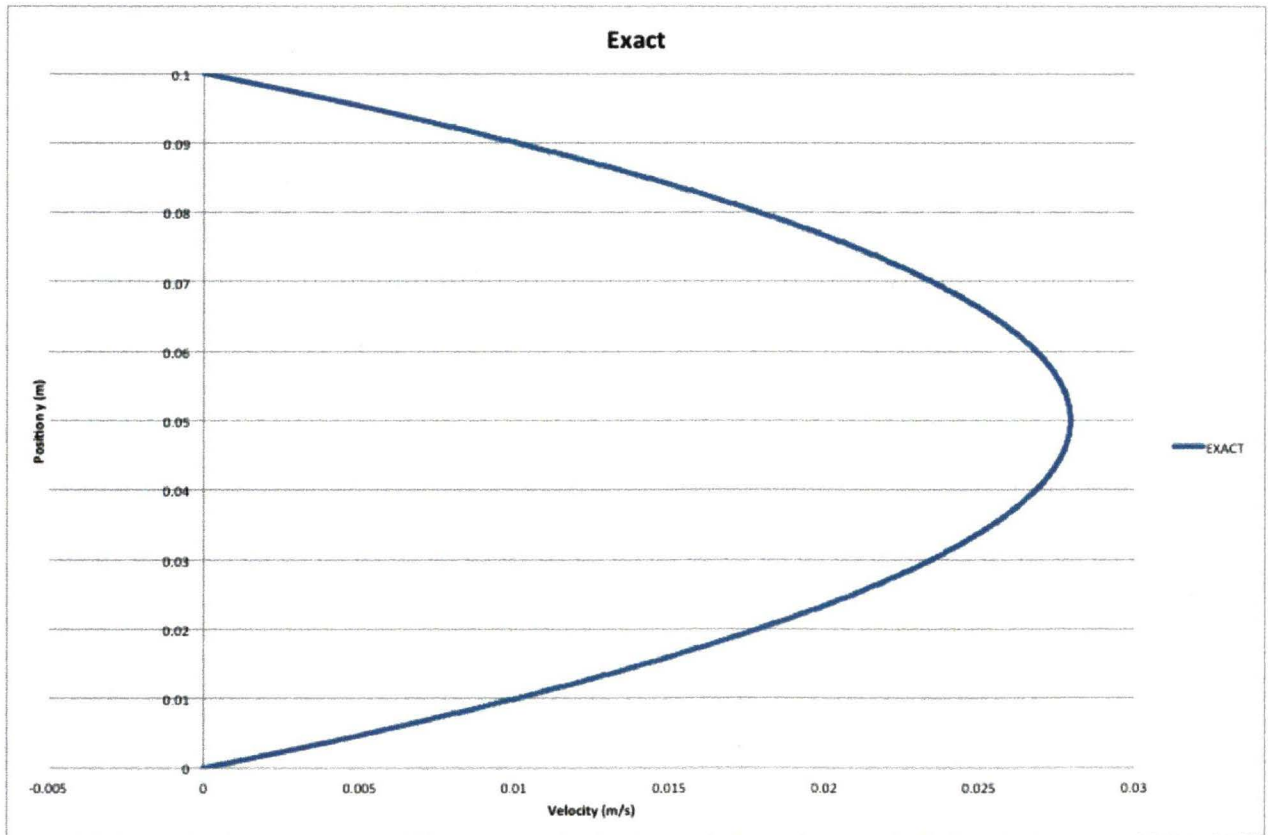


Figure 1 – Exact Solution

A CFD model was created for the same conditions and the uncertainty calculation performed as outlined in the next section.

## V. Uncertainty Calculation

The uncertainty can be calculated by expanding equation 13 for pressure, density, numerical (grid), and solver.

$$u_{val} =$$

$$k *$$

$$\left( \left( \left( \frac{\partial v}{\partial pressure} \right)^2 B_{pressure}^2 \right) + \left( \left( \frac{\partial v}{\partial rho} \right)^2 B_{rho}^2 \right) + \left( \left( \frac{\partial v}{\partial num} \right)^2 B_{num}^2 \right) + \left( \left( \frac{\partial v}{\partial solver} \right)^2 B_{solver}^2 \right) + \left( \left( \frac{\partial v}{\partial velocity} \right)^2 B_{velocity}^2 \right) \right)^{1/2} \quad (15)$$

The proposed method is to calculate the uncertainty as an oscillatory input parameter and multiply by the appropriate Student-T k-factor.

For Numerical, three grids were used and the t value of 2.92.

$$u_{val} = 2.92 * \left( \left( \left( \frac{\partial v}{\partial num} \right)^2 B_{num}^2 \right) \right)^{1/2} \quad (16)$$

$$u_{val} = 2.92 * \left| \frac{1}{2} (S_U - S_L) \right| \quad (17)$$

The centerline velocity was chosen as an example to plot, however at all points the uncertainty bands always encompass the exact solution.



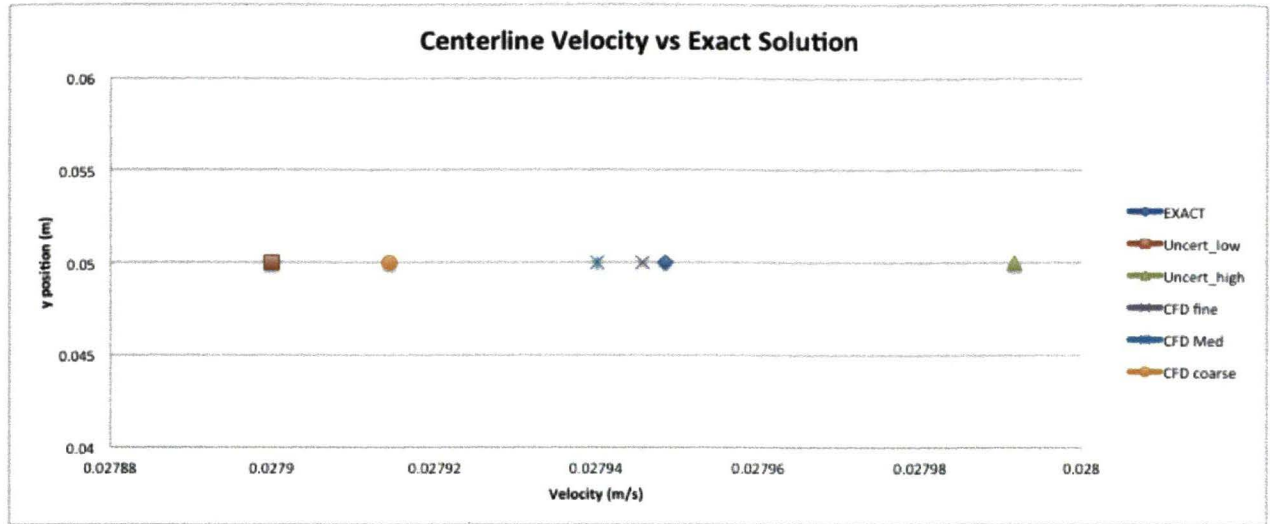


Figure 2 – Exact Solution vs. CFD with Uncertainty (Centerline Velocity) - Grid

If there is also a variation in the inlet velocity due to a tolerance or known bias, run the model at the low and high limits and use a new t-value of 2.132, which corresponds to five cases. The five cases would be three for grids and two for flow rates. A five percent variation in inlet velocity was chosen for this example.

$$u_{val} = 2.132 * \left( \left( \left( \frac{\partial v}{\partial num} \right)^2 B_{num}^2 \right) + \left( \left( \frac{\partial v}{\partial velocity} \right)^2 B_{velocity}^2 \right) \right)^{1/2} \quad (18)$$

$$u_{val} = 2.132 * \left| \frac{1}{2} (S_U - S_L) \right| \quad (19)$$

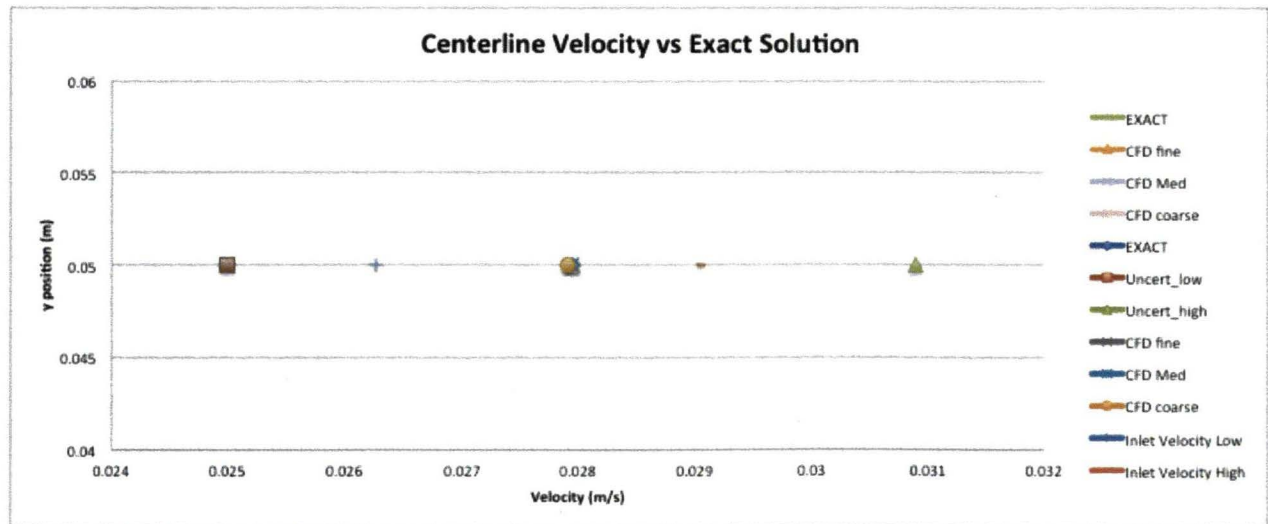


Figure 3 – Exact Solution vs. CFD with Uncertainty (Centerline Velocity) – Grid and Inlet Velocity

Also to include the outlet pressure boundary condition, run the model at the low and high known bias or tolerances and use a new t-value of 1.943, which corresponds to seven cases. The seven cases would be three for grid, two for flow rate, and two for pressure outlet boundary condition.

$$u_{val} = 1.943 * \left( \left( \left( \frac{\partial v}{\partial num} \right)^2 B_{num}^2 \right) + \left( \left( \frac{\partial v}{\partial velocity} \right)^2 B_{velocity}^2 \right) + \left( \left( \frac{\partial v}{\partial pressure} \right)^2 B_{pressure}^2 \right) \right)^{1/2} \quad (20)$$

$$u_{val} = 1.943 * \left| \frac{1}{2} (S_U - S_L) \right| \quad (21)$$

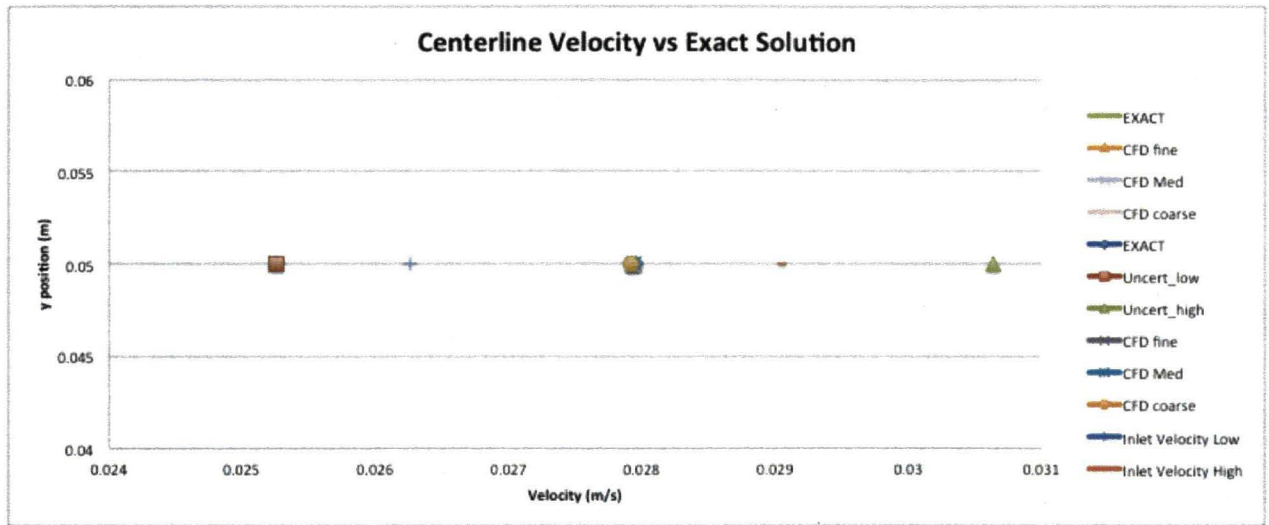


Figure 4 – Exact Solution vs. CFD with Uncertainty (Centerline Velocity) – Grid, Inlet Velocity, and Outlet Pressure

To account for the variation in fluid properties, the kinematic viscosity for air between 0 and 100 degrees Celsius is  $13.6 \times 10^{-6}$  to  $23.06 \times 10^{-6}$ . The model was run at these limits to account for the possible variation in fluid properties and a new value of  $t = 1.86$  was chosen, which corresponds to the nine cases.

$$u_{val} = 1.86 * \left( \left( \left( \frac{\partial v}{\partial num} \right)^2 B_{num}^2 \right) + \left( \left( \frac{\partial v}{\partial velocity} \right)^2 B_{velocity}^2 \right) + \left( \left( \frac{\partial v}{\partial pressure} \right)^2 B_{pressure}^2 \right) + \left( \left( \frac{\partial v}{\partial rho} \right)^2 B_{rho}^2 \right) \right)^{1/2} \quad (22)$$

$$u_{val} = 1.86 * \left| \frac{1}{2} (S_U - S_L) \right| \quad (23)$$

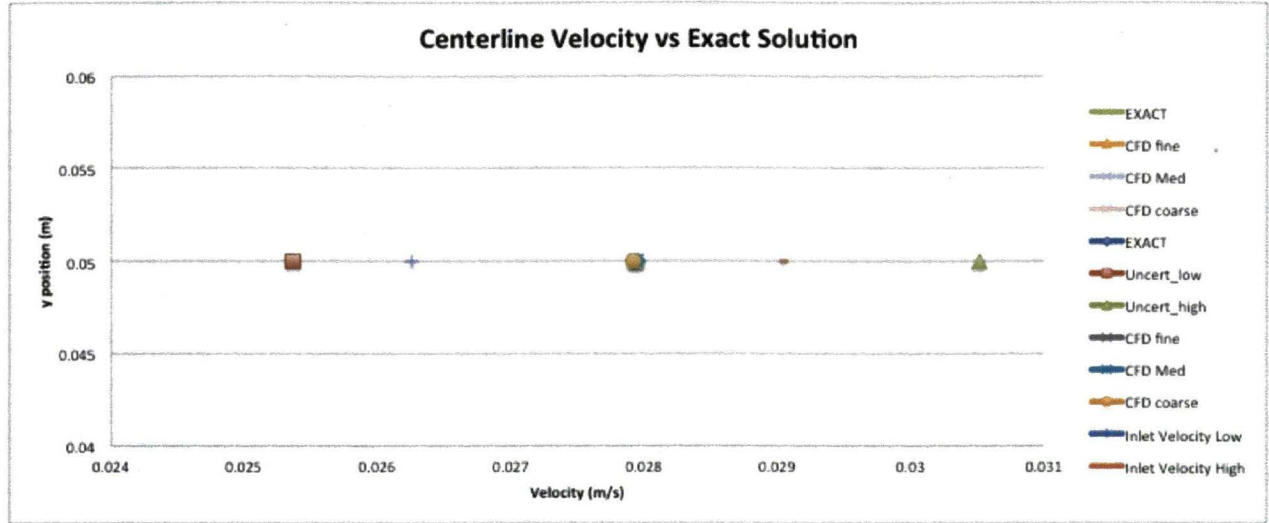


Figure 5 – Exact Solution vs. CFD with Uncertainty (Centerline Velocity) – Grid, Inlet Velocity, Outlet Pressure, and Density

Fluent has been used to calculate the results above; we also consider the solver as an input to the model. To account for the variation in the solver, the model was run in OpenFOAM. The  $t$  value was updated to 1.833 because the numbers of cases are ten.

$$u_{val} = 1.833 * \left( \left( \left( \frac{\partial v}{\partial num} \right)^2 B_{num}^2 \right) + \left( \left( \frac{\partial v}{\partial velocity} \right)^2 B_{velocity}^2 \right) + \left( \left( \frac{\partial v}{\partial pressure} \right)^2 B_{pressure}^2 \right) + \left( \left( \frac{\partial v}{\partial rho} \right)^2 B_{rho}^2 \right) + \left( \left( \frac{\partial v}{\partial solver} \right)^2 B_{solver}^2 \right)^{1/2} \quad (22)$$

$$u_{val} = 1.833 * \left| \frac{1}{2} (S_U - S_L) \right| \quad (23)$$

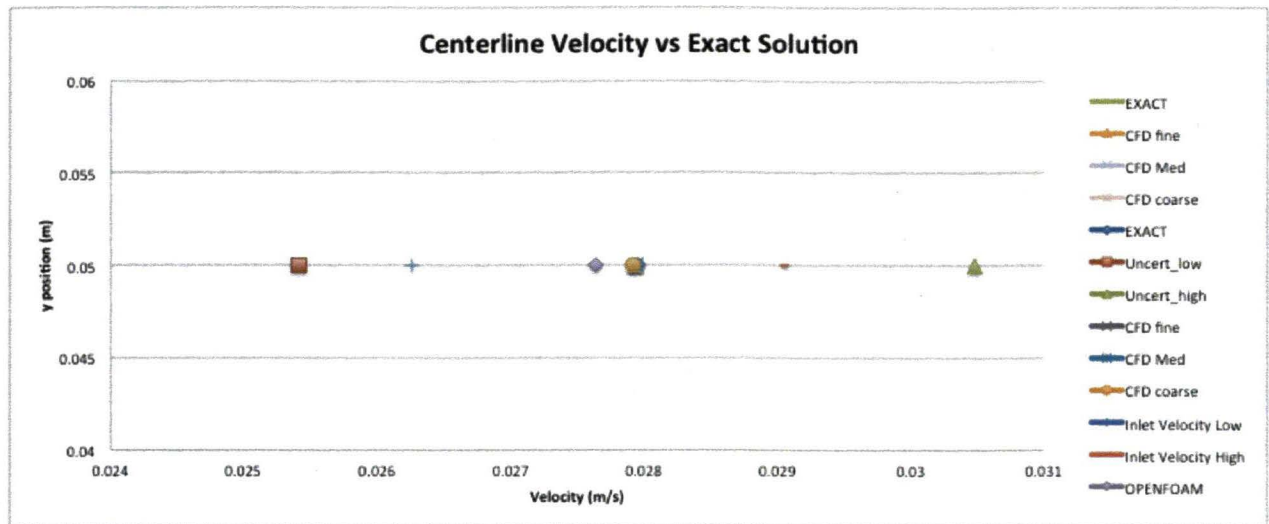


Figure 6 – Exact Solution vs. CFD with Uncertainty (Centerline Velocity) – Grid, Inlet Velocity, Outlet Pressure, Density, and Solver

Figure 7 is a plot of all the CFD cases, uncertainty, and an exact comparison.

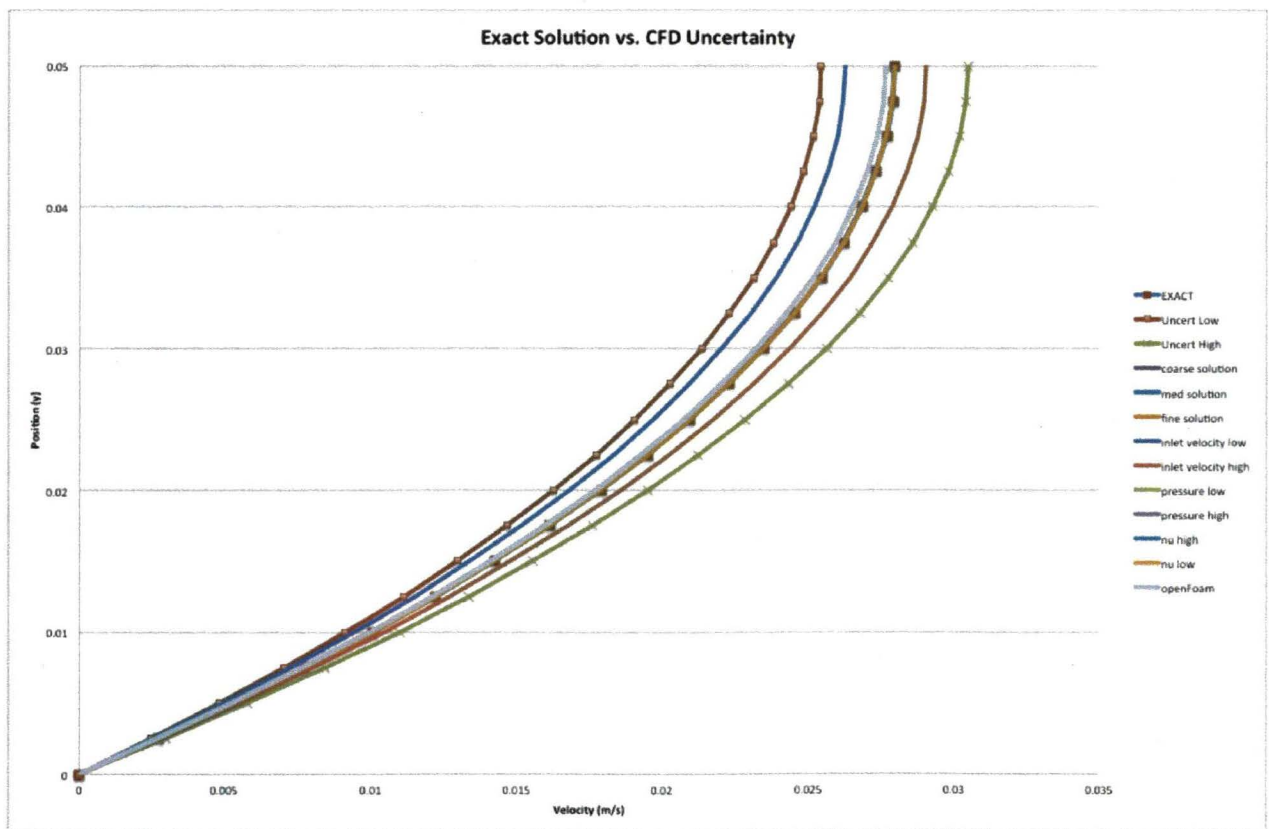


Figure 7 – Exact Solution vs. CFD with Uncertainty (Parallel Plates – Half of Domain) – Grid, Inlet Velocity, Outlet Pressure, Density, and Solver

## **VI. Conclusion**

It can be concluded that treating all inputs to a CFD model as oscillatory uncertainty parameters coupled with the Student-T distribution can supply an uncertainty estimate that encompasses the exact solution for the case considered above (fully developed, laminar, flow between stationary parallel plates). To summarize the approach and general idea, there is a standard<sup>2</sup> for calculating verification and validation of CFD using a combined numerical and experimental data. The approach described above is a way to estimate the uncertainty of a model if test data is not available. An analyst should make use of all test data that is available or able to be funded and use the ASME standard. However, if test data is missing or not attainable, the method described makes assumptions that each CFD solution belongs to an underlying Student-T distribution and a corresponding uncertainty can be estimated for a selected confidence interval.

## **References**

- [1] Groves, C., Ilie, M., Schallhorn, Paul. "Comprehensive Approach to Verification and Validation of CFD Simulations Applied to Backward Facing Step," AIAA-2013-0258, 2013.
- [2] An American National Standard., "Standard for Verification and Validation in Computational Fluid Dynamics and Heat Transfer", The American Society of Mechanical Engineers. ASME V&V 20-2009.
- [3] Stern, F., Wilson, R. V., Coleman, H. W., and Paterson, E. G., "Verification and Validation of CFD Simulations," Iowa Institute of Hydraulic Research Report No. 407, September 1999.
- [4] Fox, Robert., McDonald, Alan, "Introduction to Fluid Mechanics" 3<sup>rd</sup> Edition. John Wiley & Sons, 1985